Transmission through carbon nanotubes with polyhedral caps

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We study electron transport between capped carbon nanotubes and a substrate, and relate the transmission probability to the local density of states in the cap. Our results show that the transmission probability mimics the behavior of the density of states at all energies except those that correspond to localized states in the cap. Close proximity of a substrate causes hybridization of the localized state. As a result, transmission paths open from the substrate to nanotube continuum states via the localized states in the cap. Interference between various transmission paths gives rise to *antiresonances* in the transmission probability, with the minimum transmission equal to zero at energies of the localized states. Defects in the nanotube that are placed close to the cap cause *resonances* in the transmission probability, instead of antiresonances, near the localized energy levels. Depending on the spatial position of defects, these resonant states are capable of carrying a large current. These results are relevant to carbon nanotube based studies of molecular electronics and probe tip applications.

I. INTRODUCTION

Characteristic features of electron flow through nanotubes are relevant to both molecular electronics and experiments using nanotube tips as a probe. In these applications, the nanotube tips can be capped or open along with appropriate functionalization if desired. In preliminary studies, Dai *et al.*[1] and Wong *et al.*[2] used nanotube tips for high resolution imaging, and Wong *et al.*[3] have extended their study to include functionalized tips.[3,4] In view of such studies, which can in principle be extended to scanning tunneling microscopy (STM) measurements, it is important to understand the nature of electron flow from nanotube tips. The large number of possible topological arrangements of carbon atoms at the tip of a nanotube and the possibility of functionalizing tips makes the study of electron transport an interesting and necessary one. Further, nanotube tips have recently been observed by various authors,[5–7] and methods of constructing caps have been suggested.[8] To the best of our knowledge, electron transport through capped nanotubes have not been studied, although the local density of states (LDOS) have been studied.[5,6,9] In this paper, we study electron flow from a substrate to a nanotube tip, much like in an STM experiment where the nanotube is the tip. In this particular study, we restrict the topology of the tip to that of a polyhedral cap. The LDOS at the cap has resonances corresponding to quasi-localized states as observed experimentally in Refs. 5 and 6. In particular, Tamura *et al.*[9] have theoretically shown the existence of purely localized states in nanotubes with polyhedral caps. The effect of localized states on current flow, and the relationship between local density of states and current flow through various cap atoms are of particular interest.

Consider a nanotube interacting with a substrate as shown in Fig. 1(a). The wave functions of the cap and substrate overlap due to their physical proximity.[10] This overlap provides a physical mechanism for the hybridization of localized and continuum states, which causes the localized states (discrete energy levels) to become quasilocalized. The effect of localized states on the transmission probability in general *depends* on the nature of interaction between the localized and continuum states. Examples from the literature, which illustrate this point are a quantum well with quasilocalized levels (double barrier resonant tunneling diode) and a quantum wire with a stub containing quasilocalized levels.[11] Con-

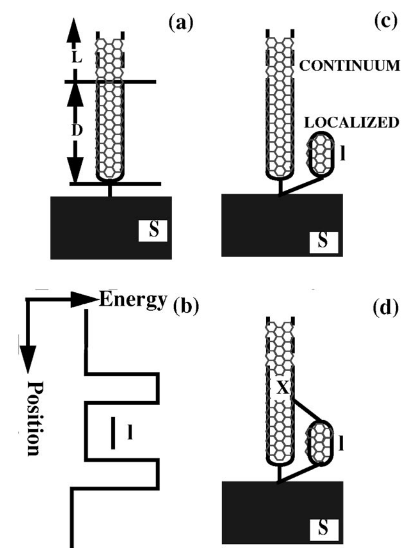

FIG. 1. (a) The CNT-substrate system is divided into three regions **S**, **D**, and **L**. (b) The potential profile versus position of a double barrier resonant tunneling structure. An electron can be transmitted from the continuum states on the top to the bottom, only via the localized state (represented by **l**) in the well. (c) In the absence of defects, the localized and continuum states in the nanotube are decoupled. In this figure, they are shown spatially separated for clarity. Coupling between the substrate and cap causes opening of transport paths where an electron incident in the substrate tunnels into and out of the localized state before being scattered into the continuum. This results in an antiresonance. (d) The presence of defects (represented by **X**) in the tube open additional transport paths similar to those in double-barrier resonant tunneling structures, with coupling to the substrate and scattering by the defect acting as the two scattering centers [compare with (b), where the two scattering centers are the barriers]. This transforms the transmission antiresonance in (c) to a resonance.

sider a quantum well with a single localized level. Let this level be coupled to continuum states both above and below as shown in Fig. 1(b). An electron incident from the continuum states on the top can be transmitted to the continuum states below only via the localized state. It is well known that the transmission probability through such a structure exhibits a resonance that corresponds to the localized state. In contrast to this example, a localized state can also interact with a continuum as shown in Fig. 1(c). The primary difference of electron transmission paths in this case when compared to the double barrier structure in Fig. 1(b) is that an electron incident in the substrate can be transmitted to the continuum states of the nanotube via paths that do not use the localized state (in a perturbative sense), in addition to paths that use the localized state. Similar transmission paths exist in the context of scattering of light from molecules,[12] electron transport through quantum wires with stubs[11] and tunneling through a heterostructure barrier.[13] In these cases, localized states play an important role in determining the transmission probability around the localized energy level. In particular, the transmission probability exhibits an antiresonance due to the localized energy level.

An isolated nanotube with a polyhedral cap has localized states in the cap that decay into the nanotube.[9] Electrons can be transmitted from the substrate to the nanotube by paths that both do and do not use the localized level. We show that the transmission probability in this case has an *antiresonance* corresponding to the energy of the localized level. This picture changes drastically if there are defects in the nanotube. Defects in the nanotube as shown pictorially in Fig. 1(d) open new transmission paths, which cause *resonances* in the transmission probability close to the localized energy levels.

We focus on the truly metallic armchair tubes, which show promise as quantum wires and for nanotube-based probes involving a tunnel current. The fivefold symmetric polyhedral cap with one pentagon at the cap center and five pentagons placed symmetrically along the edge of a (10,10) nanotube is considered (Fig. 2). The outline of the paper is as follows. In Sec. II, we describe the method used to calculate the transmission probability and density of states. In Sec. III, we study the relationship between the LDOS and electron transmission probability by addressing the following issues: (i) the relationship between LDOS and transmission probability through cap atoms, (ii) the effect of the localized energy levels in the cap (Sec. III A), (iii) a simple one dimensional model to understand the essential feature of Secs. III A and III C (Sec. III B), and (iv) the effect of defects on tunnel current/transmission probability (Sec. III C). Conclusions of this study are summarized in Sec. IV.

II. METHOD

In this section, we outline the formalism used and also discuss the assumptions made in our study. The combination of CNT and substrate can be conceptually divided into three regions: substrate (**S**), section of CNT including the cap (**D**) and a semi-infinite CNT region (**L**) as shown in Fig. 1(a). The advantage of this procedure is that the influence of the semi-infinite region **L** and the substrate can be included exactly as a selfenergy to the $[E-H]$ matrix with dimension

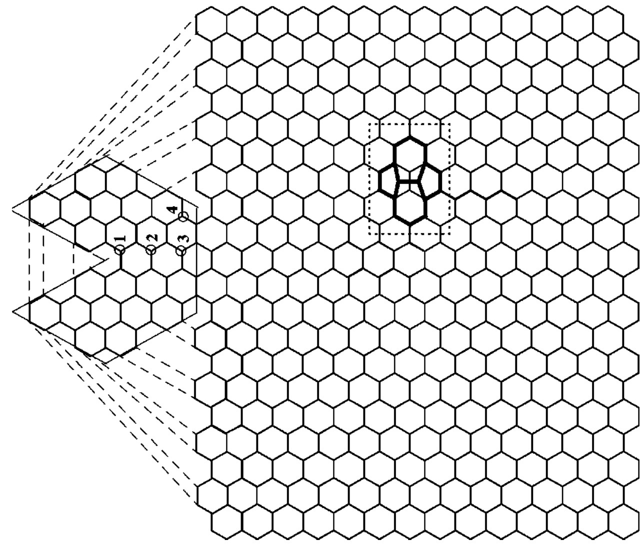

FIG. 2. (10,10) carbon nanotube with a polyhedral cap. The dashed lines connect equivalent sites of the cap and nanotube in this two dimensional representation. The dashed box shows a Stone-Wales defect.

equal to the number of atoms in **D** (H is the Hamiltonian of **D**).[14] This procedure is not sensitive to the exact location of the interface between **L** and **D** when charge self-consistency is neglected. We typically take region D to consist of five to a hundred unit cells of an armchair tube, and the results are not sensitive to the exact number as long as the retarded Green's function of region **L** (see g_L^r below) is calculated accurately. The transmission and LDOS are calculated using the method in Ref. 15. The retarded Green's function G^r is obtained by solving

$$[E-H-\Sigma_L^r(E)-\Sigma_S^r(E)]G^r(E)=I, \qquad (1)$$

where H is the sub-Hamiltonian of region **D**. $\Sigma_L^r(E) = V_{DL} g_L^r(E) V_{LD}$ is the selfenergy due to the semi-infinite region **L** that is folded into the Hamiltonian of region **D**. V_{DL} (V_{LD}) is the term in the full Hamiltonian representing the interaction between **D** (**L**) and **L** (**D**), and g_L^r is the retarded Green's function of region **L** that is calculated by assuming **L** to be isolated from **D** and **S**. The only terms of g_L^r that enter the calculation of $\Sigma_L^r(E)$ corresponds to lattice sites in **L** that are connected to **D**. That is, only the surface Green's function of **L** is required.[15] Σ_S^r is the self energy due to the substrate. In this paper, we assume Σ_S^r to be an energy-independent parameter that represents coupling between **S** and only one atom in the cap. This assumption is usually valid over small energy ranges that are away from sharp features in the substrate density of states.

The single particle LDOS at site i $[N_i(E)]$ and transmission probability $[T(E)]$ at energy E are obtained by solving Eq. (1) for the diagonal element G_{ii}^r and the corner off-diagonal submatrix of G^r whose row and column indices correspond to atoms in **D** that couple **L** and **S**, respectively:

$$N_i(E) = -\frac{1}{\pi}\mathrm{Im}[G^r_{ii}(E)] \quad (2)$$

$$T(E) = \mathrm{Trace}[\Gamma_L G^r \Gamma_S G^a]. \quad (3)$$

Γ_L and Γ_S are the coupling rates of **D** to the semi-infinite nanotube **L** and substrate **S**, respectively. $\Gamma_L = 2\pi V_{DL}\rho_L(E)V_{LD}$, where $\rho_L(E) = -(1/\pi)\mathrm{Im}[g^r_L(E)]$ is the surface density of states of **L** (Im extracts the imaginary part) and $\Gamma_S = -2\,\mathrm{Im}[\Sigma^r_S]$.

For tubes with defects, we consider the Stone-Wales model that creates two pentagon-heptagon pairs in the hexagonal network (see dashed box in Fig. 1).[16,17] Finally, the numerical calculations use the single orbital real-space tight-binding representation of the CNT Hamiltonian,[17]

$$H = -b\sum_{i\neq j} c_i^\dagger c_j + \mathrm{c.c.}, \quad (4)$$

where each carbon atom has a hopping parameter b with its three near neighbors, and c_i $(c_i^\dagger)$ is the annihilation (creation) operator at atomic site i. The value of b is chosen to be 3.1 eV.

III. RESULTS AND DISCUSSION

The main issues addressed in this section are: (i) the relationship between LDOS and transmission probability through cap atoms in a defect free CNT, (ii) the effect of localized energy levels on the transmission probability (Sec. III A), (iii) a simple one dimensional model to understand the essential features of Secs. III A and III C (Sec. III B) and, (iv) the effect of defects on tunnel current/transmission probability (Sec. III C). We only consider weak coupling between the nanotube and substrate **S**. The coupling strength (Σ^r_S) is defined to be weak if it is smaller than the value between two near neighbor carbon atoms along the length of the nanotube (diagonal elements of Σ^r_L).

A. Antiresonances in transmission probability

We first address issues (i) and (ii) involving defect free caps by studying the relationship between the LDOS at atom i in the cap and the transmission probability from the substrate to the semi-infinite CNT via atom i. An isolated polyhedral cap has localized levels (no broadening).[9] Figure 3 shows the effect of coupling of the cap to the substrate. In the calculations, one atom in the cap couples to the substrate (as labeled in Fig. 3). Coupling of the cap to the substrate causes hybridization with the substrate continuum states. As a result of hybridization, the localized states become quasilocalized, as represented by the broadened resonances in Fig. 3. In the energy range considered, there are two localized states, one around 0.25 eV and the other around -1.5 eV. The value of $\Sigma^r_S = -i\Gamma_S/2 = -12.5i$ meV for all curves in Fig. 3.

The LDOS varies significantly with atomic location. The LDOS at apex atom 1 is almost an order of magnitude smaller than the LDOS at atom 4, which is located at the cap

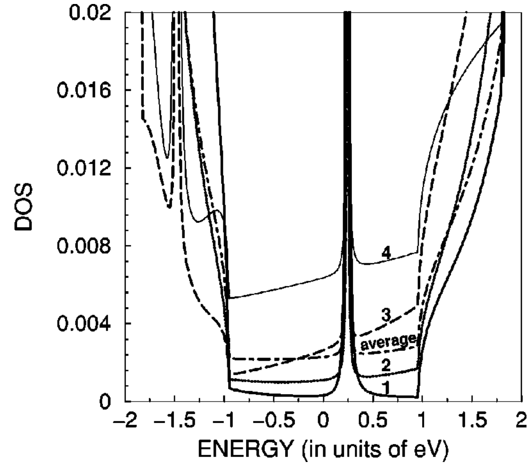

FIG. 3. The LDOS at four different cap atoms versus energy for a nanotube without defects in contact with the substrate. The LDOS is plotted at the cap atom making contact to the substrate, in the case of a defect-free nanotube [Fig. 1(c)]. The resonant peaks correspond to localized energy levels. The four curves correspond to the indexed cap atoms in Fig. 2. The legend ''average'' corresponds to the LDOS averaged over all cap atoms when atom 4 makes contact to the substrate. $\Sigma^r_S = -12.5i$ meV ($\Gamma_S = 25$ meV) for the four cases.

edge. The LDOS of atoms 2 and 3, which lie in between (see Fig. 2), and the DOS averaged over all cap atoms are also shown for comparison. The transmission probability versus energy for the cases corresponding to Fig. 3 are shown in Fig. 4. The strength of coupling in Fig. 4 is the same as in Fig. 3. The transmission probability follows the LDOS at most energies in that the magnitude is proportional to the LDOS as is seen by comparing Figs. 3 and 4. There is a major difference at the resonant energy, where *the LDOS peaks corresponds to transmission zeroes*. The transmission antiresonances arise from hybridization of localized and continuum states via coupling to the substrate as represented pictorially in Fig. 1(c). States in the CNT cap comprise of localized (ϕ_l) and continuum (ϕ_c) states that are not coupled to each other in an isolated cap. Bringing the substrate in close proximity to

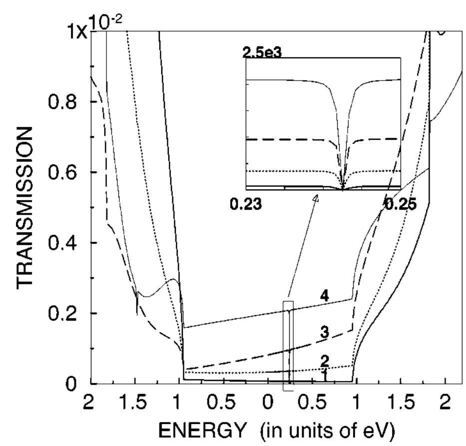

FIG. 4. The transmission probability versus energy corresponding to Fig. 3. The antiresonances occur at the same energy as the LDOS resonances in Fig. 3. The inset shows an expanded view of the antiresonances.

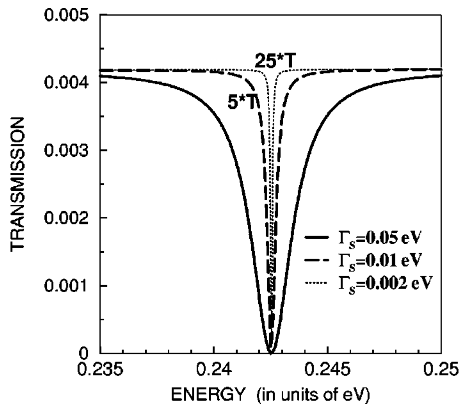

FIG. 5. The width of the antiresonance increases with increase in the strength of coupling Γ_S but the minimum is zero. The dotted and dashed curves are scaled by 25 and 5 times of the computed transmission probability respectively. In these calculations atom 4 makes contact to the substrate with a coupling strength $\Sigma_S^r = -i\Gamma_S/2$, where the values of Γ_S are given in the figure legend.

the cap couples ϕ_l and ϕ_c to the substrate states (ϕ_s). As a result, electrons have many paths to be transmitted from ϕ_s to ϕ_c: (i) directly from $\phi_s \rightarrow \phi_c$, (ii) $\phi_s \rightarrow \phi_l \rightarrow \phi_s \rightarrow \phi_c$ and (iii) higher order representations of (ii). The interference between these paths gives rise to the transmission zeroes at the resonant energies (inset of Fig. 4). The numerical calculation in this subsection is complemented by a simplified analytical model in Sec. III B to demonstrate the physics more clearly.

When the strength of coupling between the cap and substrate increases, the antiresonances becomes more pronounced. That is, the minimum is still zero but the width increases with increase in coupling strength Γ_s. To demonstrate this, atom 4 is assumed to make contact to the substrate with coupling strengths as given by the legend of Fig. 5. The real part of Σ_S^r has been assumed to be zero in Figs. 3, 4, and 5. The primary effect of including a non zero real part of Σ_S^r is to make the transmission versus energy more asymmetric. The position of the antiresonance however remains unchanged.

B. Simple one dimensional model

In this section, we present a simple one dimensional model of transport from a tip that has a localized state to a substrate, much like in Fig. 1(a). The expression for transmission coefficient is obtained analytically and aids in understanding the numerical results of Secs. III A and III C, which consider a nanotube. We now define the model. The continuum states of the tip are modeled as a one-dimensional semi-infinite chain with on-site energy ϵ_c and hopping parameter b_c (Fig. 6). The energy spectrum of such a chain has

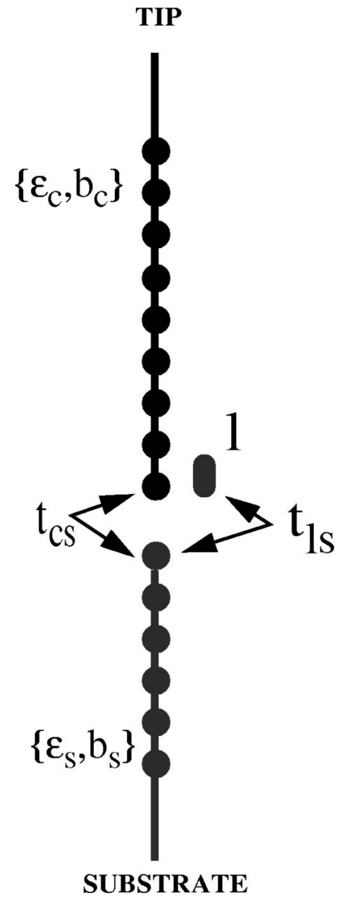

FIG. 6. A one-dimensional model describing tunneling between a tip with a localized energy level ϵ_l and a substrate. The localized level is shown separated from the atom at the edge of the tip for clarity.

a band width equal to $4b_c$ and there are no localized states in this band width. The localized level at the tip is modeled as a state with energy ϵ_l that lies spatially at the edge of the tip and energetically within the continuum of the tip states. The localized state hybridizes with the continuum states of the tip at the edge atom and this is modeled by a hopping parameter t_{lc}. The localized state ($t_{lc}=0$) of an isolated tip becomes quasilocalized when $t_{lc} \neq 0$. The substrate is also modeled as a one-dimensional semi-infinite chain with on-site potential ϵ_s and hopping parameter b_s. The substrate states hybridize with the continuum and localized states of the tip only at the tip-edge, and these are modeled by hopping parameters t_{cs} and t_{ls} respectively. The subscripts l, c, and s represent localized, continuum, and substrate states, respectively.

Following the method described in Sec. II, the retarded Green's function of the continuum and localized states at the edge of the tip are,

$$G^r(E) = D^{-1} \begin{pmatrix} E-\epsilon_l - t_{ls}^2 g_s^r(E) & t_{lc} + t_{cs} t_{ls} g_s^r(E) \\ t_{lc} + t_{cs} t_{ls} g_s^r(E) & E-\epsilon_c - t_{cs}^2 g_s^r(E) - b_c^2 g_c^r(E) \end{pmatrix}, \quad (5)$$

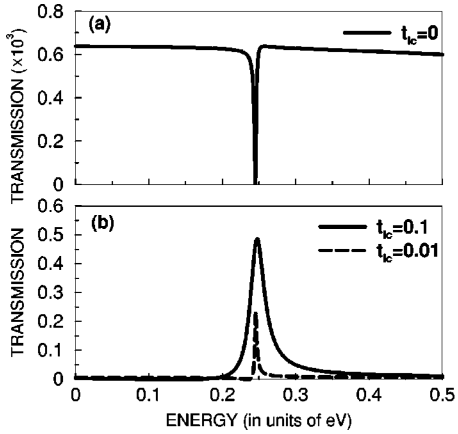

FIG. 7. (a) Transmission probability versus energy when $t_{lc}=0$ shows an antiresonance. (b) When $t_{lc}\neq 0$, the antiresonance in (a) disappears around the localized energy level and the transmission probability has a resonance. The width of this resonance decreases as t_{lc} decreases.

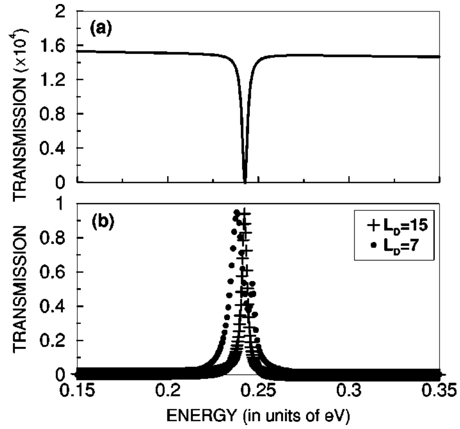

FIG. 8. (a) Transmission probability versus energy in the absence of a defect. (b) Transmission probability versus energy for the same structure in (a) but with a defect located at L_D. The strong resonance caused by an appropriately placed defect is capable of carrying large current. In these calculations, the coupling strength between atom 1 and the substrate is assumed to be $\Sigma_S^r = -25i$ meV ($\Gamma_S = 50$ meV).

where, D is the determinant of the matrix in the bracket of Eq. (5). The (1,1) and (2,2) components of $G^r(E)$ correspond to the continuum and localized states respectively, and the off-diagonal term corresponds to the correlation between the continuum and localized states. The surface Green's function of the substrate and tip chains are given by, $g_i^r = [E-\epsilon_i - \sqrt{(E-\epsilon_i)^2 - 4b_i^2}]/2b_i^2$, where $i \in c,s$.

The transmission amplitude of an electron from the substrate to the nanotube is,[14]

$$t(E) = [2\pi\rho_c(E)]^{1/2} b_c G_{11}^r(E) t_{cs} [2\pi\rho_s(E)]^{1/2} + [2\pi\rho_c(E)]^{1/2} b_c G_{12}^r(E) t_{ls} [2\pi\rho_s(E)]^{1/2}, \quad (6)$$

where, G_{11}^r and G_{12}^r are the (1,1) and (1,2) elements of the Green's function matrix (Eq. 5), and $\rho_i(E) = (-1/\pi)\mathrm{Im}[g_i^r(E)]$, where $i \in s,c$ is the surface density of states. The first term of Eq. (6) represents the path where an electron incident in the tip is transmitted to the substrate via the modified continuum states at the edge atom of the tip. The modification of the continuum states are due to interaction with the localized state and the substrate states. The second term of Eq. (6) represents the path where an electron incident in the tip is transmitted to the substrate via the localized state in the edge atom. $G_{12}^r(E)$ represents the correlation between the continuum and localized levels at the edge atom of the tip when the tip is connected to the substrate. The transmission probability ($|t(E)|^2$) then consists of interference between paths that do and do not use the localized state.

From Eqs. (5) and (6), the following three observations can be made: (i) The transmission coefficient is zero when,

$$E = \epsilon_l - t_{lc}\frac{t_{ls}}{t_{cs}}. \quad (7)$$

As mentioned in the beginning of this section, the case of a localized state corresponds to $t_{lc}=0$. Then, the transmission antiresonance is at the energy of the localized state ϵ_l. An example is shown in Fig. 7(a), where the parameters are $b_c = b_s = 1$ eV, $t_{ls} = t_{cs} = 0.04$ eV, $\epsilon_c = \epsilon_s = 0$ eV, and $\epsilon_l = 0.245$ eV. (ii) From Eq. (7), it is clear that the transmission probability has a zero in the presence of defects that cause hybridization between the localized and continuum states ($t_{lc}\neq 0$) even when the tip does not make contact to the substrate. The location of the transmission zero has however moved away from the localized energy by $-t_{lc}t_{ls}/t_{cs}$. (iii) A transmission resonance results when the localized level hybridizes with the continuum states in the tip ($t_{lc}\neq 0$). More specifically, when the hopping parameters t_{cs}, t_{ls} and t_{lc} are much smaller than b_c and b_s, the transmission probability has a resonance at an energy close to the localized energy level ϵ_l [Fig. 7(b)]. The precise location of the resonance depends on the values of the hopping parameters. The width of the resonance increases with increase in t_{lc} [Fig. 7(b)], a feature that is observed in the case of the nanotube also is discussed in the following subsection. Except for t_{lc}, the parameters used in Fig. 7(b) are the same as in Fig. 7(a).

C. Influence of defects

We now consider the changes to the antiresonance picture discussed in Sec. III A due to defects in the nanotube. The results for two different locations of a defect along the length of the nanotube and atom 1 making contact to the substrate with coupling strength $\Sigma_S^r = -i\Gamma_S/2 = -25i$ meV are shown in Fig. 8. While the defect considered here is the Stone-Wales defect (see dashed box in Fig. 1), we have also carried out similar calculations for defect models that involve a random change in the on-site potential and hopping parameter of carbon atoms located near the cap. The main conclusion of these calculations is that the results of this section do not qualitatively depend on the exact defect model as long as the defect hybridizes the localized and continuum states of the nanotube.

Scattering due to the defect opens up more channels for hybridization of the localized state. As a result, the LDOS of the cap will show broadened resonances similar to those in

Fig. 3. The transmission probability changes significantly around the localized energy levels in comparison to Fig. 4, as shown in Fig. 8. The sharp transmission antiresonances at the localized energy has disappeared and instead the transmission probability has resonances around the energy of the localized state. This is because the defect locally mediates mixing/hybridization of localized and continuum states. As a result, the localized states are coupled to continuum states by two scattering centers: the defect in the nanotube and the interaction with the substrate. This leads to additional transmission paths that are similar in spirit to paths in a double barrier resonant tunneling structure in Fig. 1(b), where the two scattering centers are the barriers. The simple model discussed in Sec. III B also demonstrates this point [Fig. 7 and discussion of (iii) at the end of Sec. III B].

The resonance width of the transmission probability is determined by two contributions. The first contribution is the hybridization due to the substrate and the second contribution is the hybridization due to the defect. The second contribution depends on $|\langle \phi_C | H_{defect} | \phi_L \rangle|$, where H_{defect} is Hamiltonian of the defect. Figure 8 shows the transmission probability for two different distances of the defect from the cap (L_D). L_D equal to 7 and 15 are in units of the one-dimensional unit-cell length of armchair tubes. The main feature is that the width becomes smaller as distance of the defect from the cap increases. This trend can be understood from the fact that $|\phi_L|^2$ (or the density of states of the localized state) decays with distance away from the cap. As a result, the strength of hybridization between continuum and localized states in the cap arising due to the defect $[|\langle \phi_C | H_{defect} | \phi_L \rangle|]$ decreases as distance of the defect from the cap apex increases. This corresponds to t_{lc} becoming smaller in the model discussed in Sec. III B [see discussion of (iii) at the end of Sec. III B].

IV. CONCLUSIONS

We studied phase coherent transport through carbon nanotube tips in proximity to a substrate. An armchair tube with a polyhedral cap has localized states that decay with distance away from the cap. We find that these localized states play an important role in determining the features of the electron transmission probability from the substrate to the nanotube. The transmission probability corresponds directly to the LDOS at energies away from the localized energy levels. Close to the localized energy level, while the LDOS exhibits a resonance, the transmission probability exhibits an antiresonance. Defects in the tube alter the antiresonance by providing additional defect-assisted channels for transport into the continuum states of the CNT. As a result, the transmission probability has a resonance close to the localized energy levels, instead of an antiresonance. These resonances are capable of carrying a large amount of current compared to other energies, and so are relevant to experiments that measure the tunnel current using carbon nanotube-based tips. The current carrying capacity of the resonance depends on two parameters: the hybridization strengths of the localized state due to interaction with the substrate, and defect assisted interaction with the continuum states of the nanotube. Since the density of states of the localized levels decay with distance into the nanotube, the hybridization strength due to defect assisted scattering decreases. The current carrying capacity of the resonances then decreases with increase in the distance of the defect from the cap.

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